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# EIC 1700 SEARCH REQUEST

Today's Date 5-14-68

Name Sin J. Lee

AU/Org. 1795 Examiner # 76060

Bld.&Rm.# Rem. Phone 2-1333  
(905)

Priority App. Filing Date P/z. See B-16

Case/App. # 10/527,068

## Format for Search Results

EMAIL \_\_\_\_\_ PAPER \_\_\_\_\_

If this is a Board of Appeals case, check here ☐

## Synonyms

SCIENTIFIC REFERENCE BR  
Sci & Tech Inf Cntr

MAY 15 RECD

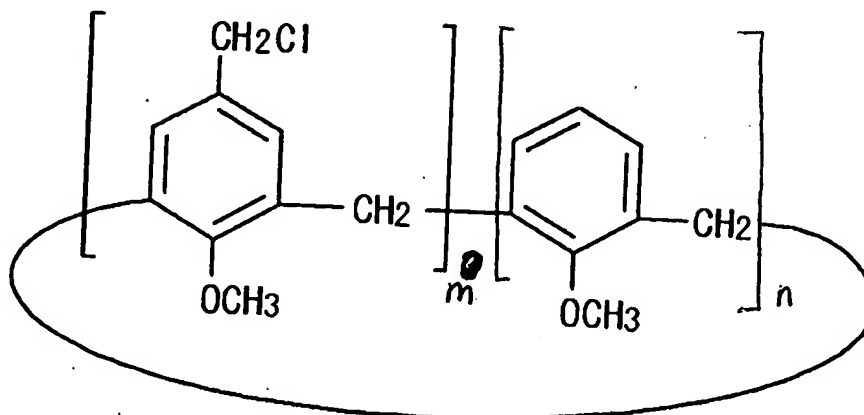
Describe this invention in your own words.

Pat. &amp; T.M. Office

## Terms to avoid

### Additional Comments

Final Comments Plz. search for a resist composition containing the following compound


$$m = 1-3$$

(II)

Please submit complete

**STAFF USE ONLY**

### Type of Source

\*\*\*\*\*

### Abstract

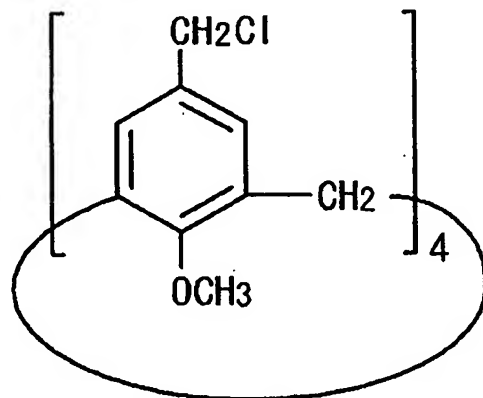
The resist according to the present invention includes any one of tetrachloromethyl tetramethoxycalix [4] arene and trichloromethyl  
5 tetramethoxycalix [4] arene. The resist including such kind of components is soluble in the solvent having less effect to worsen a working environment, namely, ethyl lactate (EL), propylene glycol monomethyl ether (PGME), propylene glycol monomethyl ether acetate  
10 (PGMEA), ethyl propionate, n-butyl acetate and 2-heptanone. It can be developed by tetra-methyl ammonium hydroxide in addition to the above mentioned solvent. By exposing this resist by electronic ray, high resolution of 8 nm is attained, and by using this  
15 resist as a mask, various materials can be formed into a hyperfine shape. According to such kind of resist, a photosensitive resist material which has high resolution and solvable to solvents having less effect to worsen the working environment and can be developed  
20 by the solvents, a exposure method using it, and a hyperfine processing method using it are provided.

**AMENDMENTS TO THE CLAIMS**

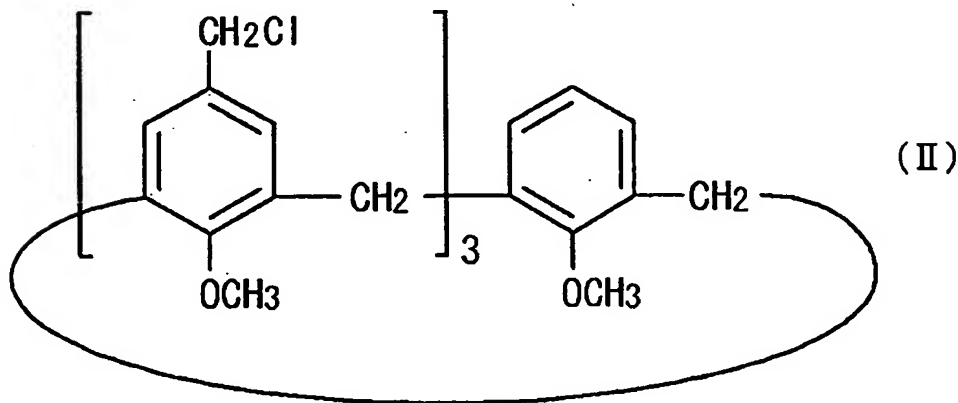
1. (Canceled)

2. (Original) A resist comprising at least one of 5,11,17,23 - tetrachloromethyl - 25,26,27,28 - tetramethoxycalix [4] arene (CMC4AOMe) represented by the structural formula (I) of the following chemical formula 3 and 5,11,17 - trichloromethyl - 25,26,27,28 - tetramethoxycalix [4] arene (CMC3AOMe) represented by the structural formula (II) of the following chemical formula 4.

[Chemical Formula 3]

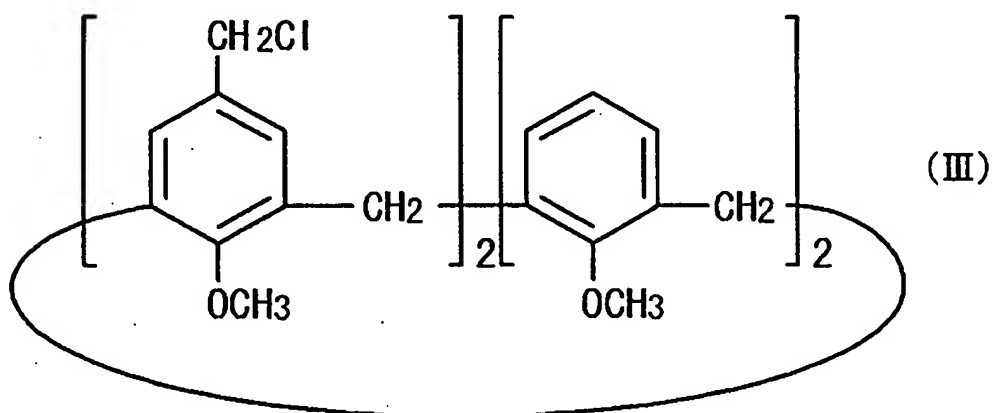


[Chemical Formula 4]

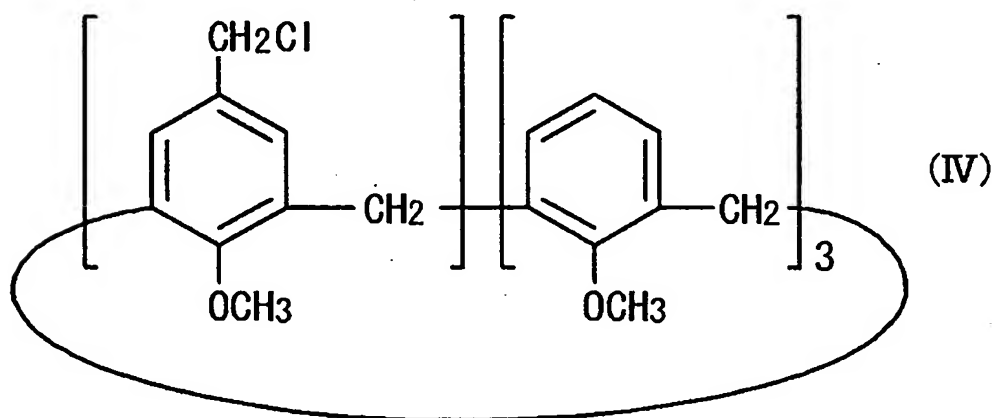


3. (Original) The resist according to claim 2, further comprising at least one of 5,11 – dichloromethyl – 25,26,27,28 – tetramethoxycalix [4] arene (CMC2AOMe) represented by the structural formula (III) of the following chemical formula 5 and 5 – monochloromethyl – 25,26,27,28 – tetramethoxycalix [4] arene (CMC1AOMe) represented by the structural formula (IV) of the following chemical formula 6 is provided.

[Chemical Formula 5]



[Chemical Formula 6]



4. (Previously Presented) The resist according to claim 2, further comprising at least one of oligomer and organic polymer compound.

5. (Previously Presented) The resist according to claim 2, which is exposed by the irradiation of at least one of electronic beam, X-ray, ion beam and atomic beam.

6. (Previously Presented) The resist according to claim 2, further comprising, at least one solvent selected from the group consisting of ethyl lactate (EL), propylene glycol monomethyl ether (PGME), propylene glycol monomethyl ether acetate (PGMEA), ethyl propionate, n-butyl acetate and 2-heptanone.

7. (Original) A method for forming a resist pattern comprising the following steps of coating the resist according to claim 6 on a substrate, exposing said resist to a radioactive ray; and a step developing said resist.

8. (Original) The method according to claim 7,  
Wherein said radioactive ray is any of electronic beam, X-ray, ion beam and atomic beam.

9. (Previously Presented) The method according to claim 7,  
wherein said developing step is carried out by using a developer comprising at least one selected from the group consisting of ethyl lactate (EL), propylene glycol monomethyl ether

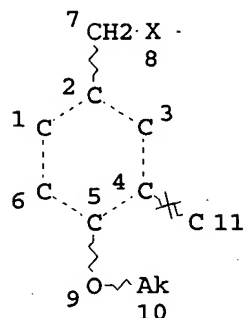
(PGME), propylene glycol monomethyl ether acetate (PGMEA), ethyl propionate, n-butyl acetate, 2-heptanone and tetramethyl ammonium hydroxide.

10. (Previously Presented) A method for hyperfine processing comprising the steps of forming a resist pattern using the resist pattern forming method according to claim 7; and performing a processing on said substrate with said resist pattern as a mask.

11. (Previously Presented) The resist according to claim 3, further comprising at least one of oligomer and organic polymer compound.

=&gt; d que 125

L12 STR



## NODE ATTRIBUTES:

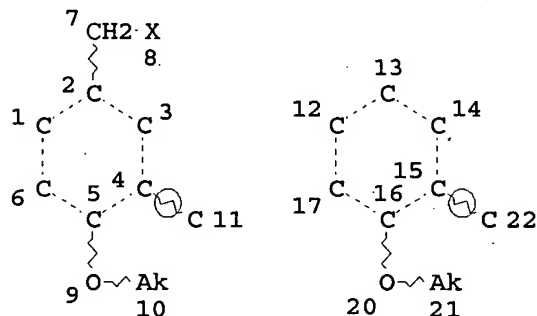
NSPEC IS RC AT 11  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 11

## STEREO ATTRIBUTES: NONE

L14 528 SEA FILE=REGISTRY SSS FUL L12  
 L19 STR



## NODE ATTRIBUTES:

NSPEC IS R AT 11  
 NSPEC IS R AT 22  
 CONNECT IS E2 RC AT 13  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

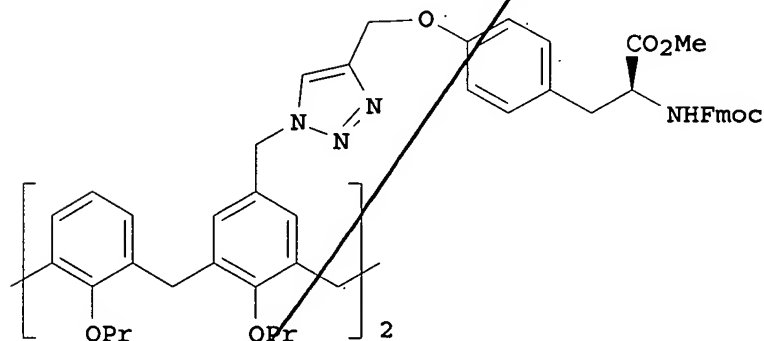
RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 20

## STEREO ATTRIBUTES: NONE

L21 19 SEA FILE=REGISTRY SUB=L14 SSS FUL L19  
 L22 16 SEA FILE=REGISTRY ABB=ON PLU=ON L21 NOT ( ISOBENZOFURANON  
 E OR PYRAN-6-ONE)  
 L25 24 SEA FILE=HCAPLUS ABB=ON PLU=ON L22

=&gt; d 125 1-24 ibib ed abs hitstr hitind

L25 ANSWER 1 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:899556 HCAPLUS  
 DOCUMENT NUMBER: 147:385707  
 TITLE: Upper Rim Appended Hybrid Calixarenes via Click Chemistry  
 AUTHOR(S): Bew, Sean P.; Brimage, Rebecca A.; L'Hermite, Nathalie; Sharma, Sunil V.  
 CORPORATE SOURCE: School of Chemical Sciences Pharmacy, University of East Anglia, Norwich, NR4 7TJ, UK  
 SOURCE: Organic Letters (2007), 9(19), 3713-3716  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 147:385707  
 ED Entered STN: 15 Aug 2007  
 GI



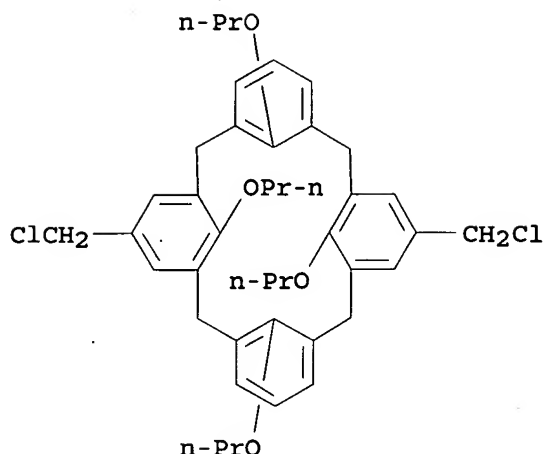
AB We report the application of "click" chemical for the synthesis of hybrid calixarenes appended on the upper rim with carbohydrate and N,C-protected  $\alpha$ -amino acids, e.g., I. The chemoselective N- or C-deprotection of the  $\alpha$ -amino acids and their subsequent transformation into dipeptides is described. The first example of a chemo-enzymic synthesis on upper rim derived calix[4]arenes using trans-sialidase affords sialylated lactose calix[4]arenes. Our innovative chemo-enzymic process paves the way for further applications.

IT 176098-86-5  
 (preparation of hybrid calixarenes appended on the upper rim with carbohydrate or protected  $\alpha$ -amino acids via copper catalyzed microwave assisted Click chemical)

RN 176098-86-5 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA  
 INDEX NAME)





CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 28, 33, 34

IT 10065-72-2, L-Alanine methyl ester 13139-15-6 34272-02-1  
125376-33-2 176098-86-5 325814-49-1 910479-36-6  
949894-57-9 949894-83-1 949894-88-6 949894-90-0 949894-92-2  
949894-99-9

(preparation of hybrid calixarenes appended on the upper rim with carbohydrate or protected  $\alpha$ -amino acids via copper catalyzed microwave assisted Click chemical)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:844150 HCAPLUS

DOCUMENT NUMBER: 145:438841

TITLE: Catalysis of Diribonucleoside Monophosphate Cleavage by Water Soluble Copper(II) Complexes of Calix[4]arene Based Nitrogen Ligands

AUTHOR(S): Cacciapaglia, Roberta; Casnati, Alessandro; Mandolini, Luigi; Reinhoudt, David N.; Salvio, Riccardo; Sartori, Andrea; Ungaro, Rocco

CORPORATE SOURCE: Dipartimento di Chimica and IMC - CNR Sezione Meccanismi di Reazione, Universita La Sapienza, Rome, 00185, Italy

SOURCE: Journal of the American Chemical Society (2006), 128(37) 12322-12330

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:438841

ED Entered STN: 24 Aug 2006

AB Calix[4]arenes functionalized at the 1,2-, 1,3-, and 1,2,3-positions of the upper rim with [12]ane-N<sub>3</sub> ligating units were synthesized, and their bi- and trimetallic zinc(II) and copper(II) complexes were investigated as catalysts in the cleavage of phosphodiester as RNA models. The results of comparative kinetic studies using monometallic controls indicate that the subunits of all of the zinc(II) complexes and of the 1,3-distal bimetallic copper(II) complex act as essentially independent mono-metallic catalysts. The lack of cooperation between

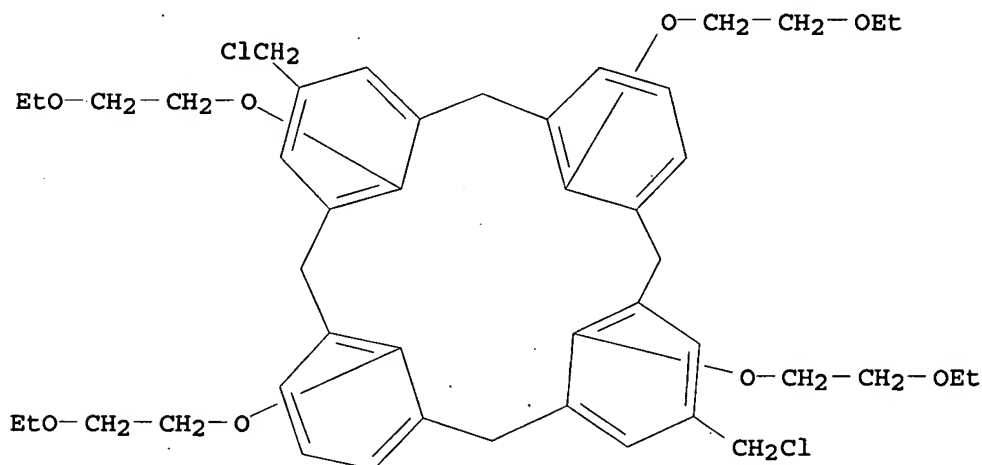
metal ions in the above complexes is in marked contrast with the behavior of the 1,2-vicinal bimetallic copper(II) complex, which exhibits high catalytic efficiency and high levels of cooperation between metal ions in the cleavage of HPNP and of diribonucleoside monophosphates NpN'. Rate accelerations relative to the background (1.0 mM catalyst, water solution, pH 7.0, 50 °C) are on the order of 10<sup>4</sup>-fold, largely independent of the nucleobase structure, with the exception of the cleavage of diribonucleoside monophosphates in which the nucleobase N is uracil, namely UpU and UpG, for which rate enhancements rise to 10<sup>5</sup>-fold. The rationale for the observed selectivity is discussed in terms of deprotonation of the uracil moiety under the reaction conditions and complexation of the resulting anion with one of the copper(II) centers.

IT 166665-14-1 426836-42-2 656242-99-8  
842171-98-6

(catalysis of diribonucleoside monophosphate cleavage by water soluble copper complexes of calixarene based nitrogen ligands)

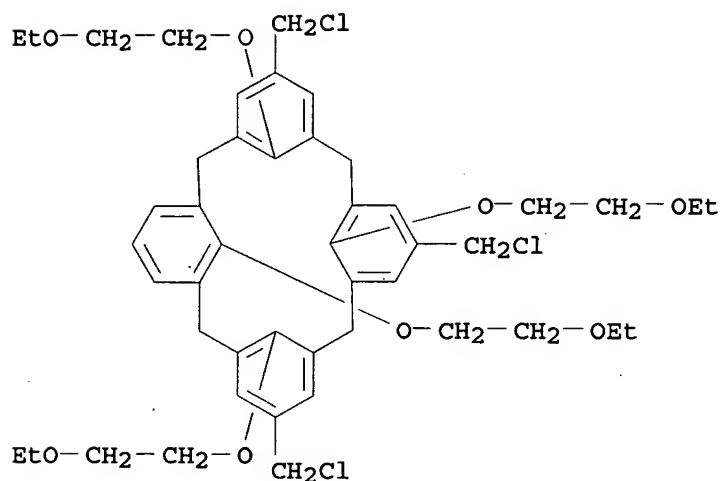
RN 166665-14-1 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy)- (CA  
INDEX NAME)

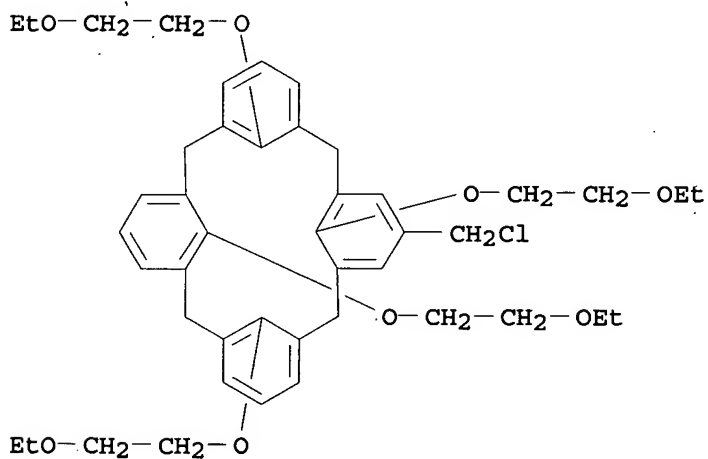


RN 426836-42-2 HCAPLUS

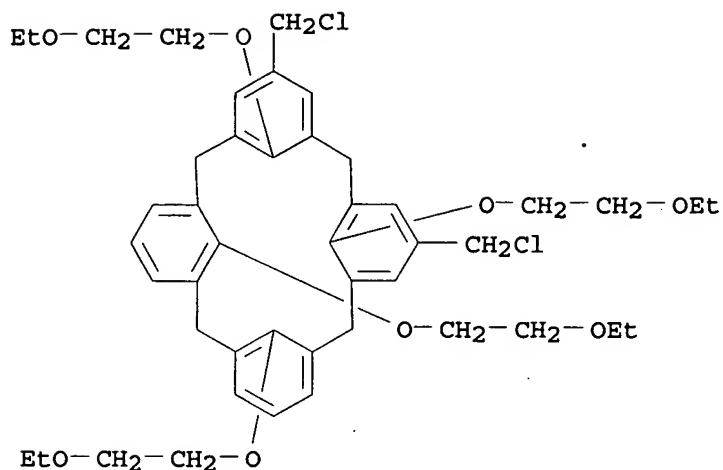
CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,11,17-tris(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy)- (CA  
INDEX NAME)



RN 656242-99-8 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5-(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy) - (CA INDEX  
 NAME)



RN 842171-98-6 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,11-bis(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy) - (CA  
 INDEX NAME)



CC 33-9 (Carbohydrates)

Section cross-reference(s): 22, 25, 78

IT 830-03-5 2382-65-2 2382-66-3 2415-43-2 2536-99-4 3352-23-6  
 3353-33-1 3474-04-2 4281-46-3 4785-07-3 6554-00-3  
 166665-14-1 174192-40-6 426836-42-2  
 656242-99-8 842171-98-6

(catalysis of diribonucleoside monophosphate cleavage by water soluble copper complexes of calixarene based nitrogen ligands)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:384572 HCAPLUS

DOCUMENT NUMBER: 145:83266

TITLE: Influence of the number and geometry of binding sites on host-guest affinity: imidazolium-substituted receptor molecules for small inorganic anions

AUTHOR(S): Fahlbusch, Tilmann; Frank, Markus; Schatz, Juergen; Schmaderer, Harald

CORPORATE SOURCE: Division of Organic Chemistry I, University of Ulm, Ulm, 89081, Germany

SOURCE: European Journal of Organic Chemistry (2006), (8), 1899-1903

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:83266

ED Entered STN: 27 Apr 2006

AB The influence of the number and relative geometry of the binding sites on the binding of spherical and tetragonal inorg. anions (Cl<sup>-</sup>, Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, and HSO<sub>4</sub><sup>-</sup>) has been studied by using imidazolium salts based on benzene and calix[4]arenes. Binding consts. in DMSO were in the range of 200-2000 L mol<sup>-1</sup>. Three or four binding sites lead to the nonselective binding of all anions indicating the decisive influence of the number of possible binding positions; binding consts. of .apprx. 2000 for H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, 1000 for HSO<sub>4</sub><sup>-</sup>, 900 for Cl<sup>-</sup>, and 800 L mol<sup>-1</sup> for Br<sup>-</sup> were obtained. Benzene and calixarene-based (5b) bis(imidazolium)

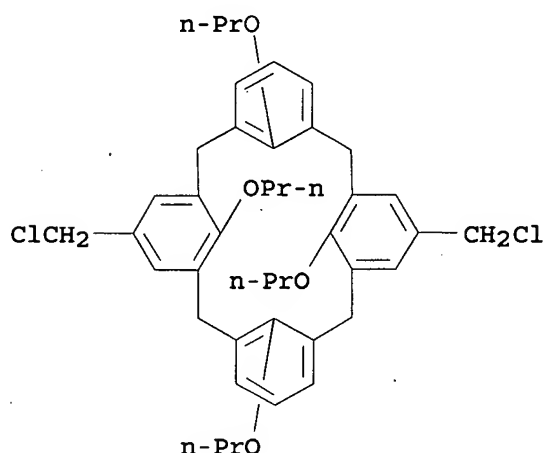
salts exhibited a high selectivity towards  $\text{H}_2\text{PO}_4^-/\text{HSO}_4^-$  and  $\text{Cl}^-/\text{Br}^-$  indicating that for the complexation of  $\text{H}_2\text{PO}_4^-$  and  $\text{Cl}^-$  two binding sites are necessary, and for  $\text{Br}^-$  and  $\text{HSO}_4^-$  at least three. In this case, selectivity could be obtained by simple variation of the number of identical binding positions.

IT 176098-86-5

(preparation and influence of the number and geometry of binding sites on host-guest affinity in imidazolium-substituted receptor mols. for small inorg. anions)

RN 176098-86-5 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA  
INDEX NAME)



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 616-47-7, 1-Methylimidazole 18226-42-1, 1,3,5-  
Tris(bromomethyl)benzene 21988-87-4, 1,3,5-Tris(bromomethyl)-2,4,6-  
trimethylbenzene 176098-86-5 190779-61-4 325814-49-1

(preparation and influence of the number and geometry of binding sites on host-guest affinity in imidazolium-substituted receptor mols. for small inorg. anions)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L25 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:44975 HCAPLUS

DOCUMENT NUMBER: 144:292271

TITLE: Kinetic Acidity of Supramolecular Imidazolium  
Salts-Effects of Substituent, Preorientation, and  
Counterions on H/D Exchange Rates

AUTHOR(S): Fahlbusch, Tilmann; Frank, Markus; Schatz,  
Juergen; Schuehle, Daniel T.

CORPORATE SOURCE: Division of Organic Chemistry I, University of  
Ulm, Ulm, D-89069, Germany

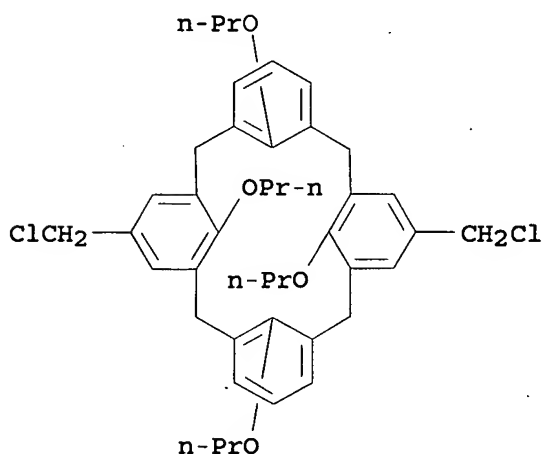
SOURCE: Journal of Organic Chemistry (2006), 71(4),  
1688-1691

CODEN: JOCEAH; ISSN: 0022-3263

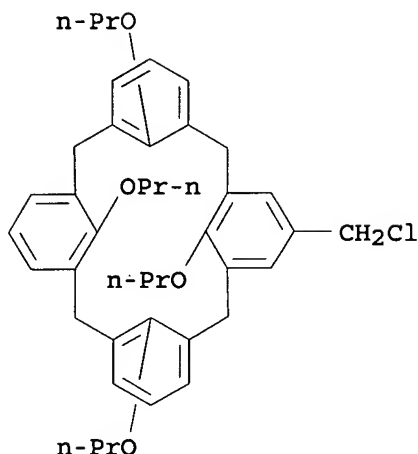
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:292271  
 ED Entered STN: 18 Jan 2006  
 AB The deprotonation of imidazolium salts to N-heterocyclic carbenes is often a decisive step in modern catalytic reactions. Therefore, we studied the H/D exchange of the C2 H of 15 imidazolium-substituted calix[4]arenes and 11 nonmacrocyclic model compds. in methanol/water (97:3). The influence of the counterion, substitution directly on the imidazolium unit or on the preorienting calixarene backbone could be studied. The observed exchange rates might give a rational for the suitability of the imidazolium salts as precursors in the Suzuki coupling.  
 IT 176098-86-5 878482-79-2  
 (quaternization reaction; substituent, preorientation, and counterions effects on H/D exchange rates and kinetic acidity of supramol. imidazolium salts)  
 RN 176098-86-5 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA INDEX NAME)



RN 878482-79-2 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 5-(chloromethyl)-25,26,27,28-tetrapropoxy- (CA INDEX NAME)



CC 22-12 (Physical Organic Chemistry)  
 IT 616-47-7, 1-Methylimidazole 25364-44-7, 1-Mesitylimidazole  
 45676-04-8, 1-tert-Butylimidazole 176098-86-5 325814-49-1  
 878482-79-2

(quaternization reaction; substituent, preorientation, and counterions effects on H/D exchange rates and kinetic acidity of supramol. imidazolium salts)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:252184 HCAPLUS  
 DOCUMENT NUMBER: 144:117657  
 TITLE: Comparative study of calixarene and HSQ resist systems for the fabrication of sub-20nm MOSFET device demonstrators  
 AUTHOR(S): Kretz, J.; Dreeskornfeld, L.; Ilicali, G.; Lutz, T.; Weber, W.  
 CORPORATE SOURCE: Corporate Research, Infineon Technologies AG, Munich, D-81730, Germany  
 SOURCE: Microelectronic Engineering (2005), 78-79, 479-483  
 CODEN: MIENEF; ISSN: 0167-9317  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

ED Entered STN: 24 Mar 2005

AB' For the fabrication of future MOSFET device demonstrators with electron beam lithog. neg. resists with target resols. smaller than 20 nm are needed. Calixarenes and hydrogen-silesquioxane are commonly used resists at present for this critical dimension (CD). We have compared two organic calixarene derivs., 4-methyl-acetoxy-calix-6-arene and chloro-methyl-tetrakis-methoxy-calix-4-arene and the inorg. low-k material hydrogen-silesquioxane in terms of their compatibility to standard CMOS processes. Resist thicknesses of 50-150 nm have been produced with both types of resist with different dilns. Contrasts are 1.8 for both calixarenes, with a clearing dose of 1200  $\mu\text{C}/\text{cm}^2$  for calix-6-arene and 330  $\mu\text{C}/\text{cm}^2$  for calix-4-arene. The contrast of 2.3 at 67  $\mu\text{C}/\text{cm}^2$  for HSQ could be increased to 3.3 by use of Choline developer instead of TMAH. Dose dependence on linewidth has been studied in detail. Etching selectivities of 4:1 for calixarene

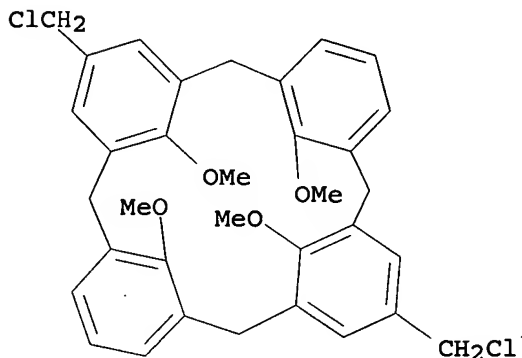
to TEOS in a fluorine gas mixture and 14:1 of densified HSQ to Si in an HBr/O<sub>2</sub> plasma have been achieved.

IT 125065-73-8

(comparative study of calixarene and HSQ resist systems for fabrication of sub-20-nm MOSFET device demonstrators)

RN 125065-73-8 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)



CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 125065-73-8 141137-71-5

(comparative study of calixarene and HSQ resist systems for fabrication of sub-20-nm MOSFET device demonstrators)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1141981 HCAPLUS

DOCUMENT NUMBER: 142:218818

TITLE: Di- and Trinuclear Zn<sup>2+</sup> Complexes of Calix[4]arene Based Ligands as Catalysts of Acyl and Phosphoryl Transfer Reactions

AUTHOR(S): Cacciapaglia, Roberta; Casnati, Alessandro; Mandolini, Luigi; Reinhoudt, David N.; Salvio, Riccardo; Sartori, Andrea; Ungaro, Rocco

CORPORATE SOURCE: Dipartimento di Chimica and IMC-CNR Sezione Meccanismi di Reazione, Universita di Roma La Sapienza, Rome, 00185, Italy

SOURCE: Journal of Organic Chemistry (2005), 70(2), 624-630

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

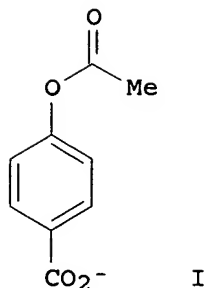
LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:218818

ED Entered STN: 28 Dec 2004

GI





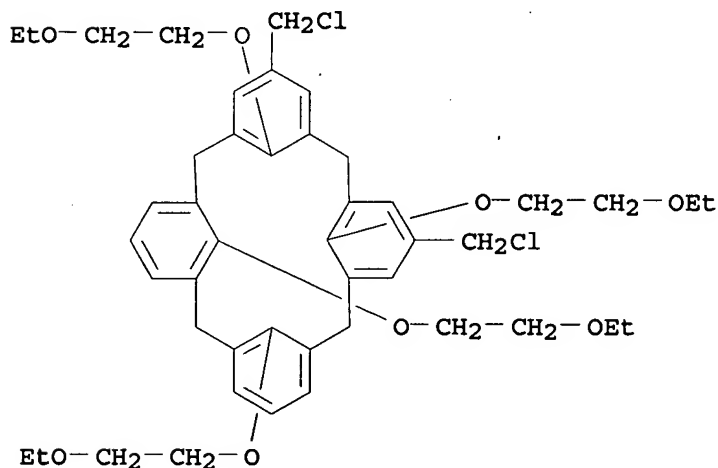
AB The calix[4]arene scaffold, blocked in the cone conformation by proper alkylation of the lower rim hydroxyls, was used as a convenient mol. platform for the design of bi- and trimetallic Zn<sup>2+</sup> catalysts. The catalytic activity of the Zn<sup>2+</sup> complexes of calix[4]arenes decorated at the 1,2-, 1,3-, and 1,2,3-positions of the upper rim with 2,6-bis[(dimethylamino)methyl]pyridine units were studied in the cleavage of ester I and of the RNA model compound HPNP. High rate enhancements, up to 4 orders of magnitude, were observed in a number of catalyst-substrate combinations. The order of catalytic efficiency among regioisomeric dinuclear complexes in the cleavage of ester I is 1,2-vicinal » 1,3-distal, but it is reversed in the reaction of HPNP. The higher efficiency of trinuclear compared to dinuclear complexes provides an indication of the cooperation of three Zn<sup>2+</sup> ions in the catalytic mechanism.

IT 842171-98-6P

(di- and trinuclear Zn<sup>2+</sup> complexes of calix[4]arene based ligands as catalysts of acyl and phosphoryl transfer reactions)

RN 842171-98-6 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosal-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 5,11-bis(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy) - (CA INDEX NAME)



CC 22-4 (Physical Organic Chemistry)  
Section cross-reference(s): 3, 7, 29, 67, 78

IT 842171-98-6P 842171-99-7P 842172-00-3P 842172-01-4P  
(di- and trinuclear Zn<sup>2+</sup> complexes of calix[4]arene based ligands)

as catalysts of acyl and phosphoryl transfer reactions)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L25 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:818945 HCAPLUS

DOCUMENT NUMBER: 142:6081

TITLE: Dinuclear barium(II) complexes based on a  
calix[4]arene scaffold as catalysts of acyl  
transfer

AUTHOR(S): Cacciapaglia, Roberta; Casnati, Alessandro; di  
Stefano, Stefano; Mandolini, Luigi; Paolemili,  
Daniele; Reinhoudt, David N.; Sartori, Andrea;  
Ungaro, Rocco

CORPORATE SOURCE: IMC CNR Sezione Meccanismi di Reazione and  
Dipartimento di Chimica, Universita La Sapienza,  
Rome, 00185, Italy

SOURCE: Chemistry--A European Journal (2004), 10(18),  
4436-4442

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:6081

ED Entered STN: 07 Oct 2004

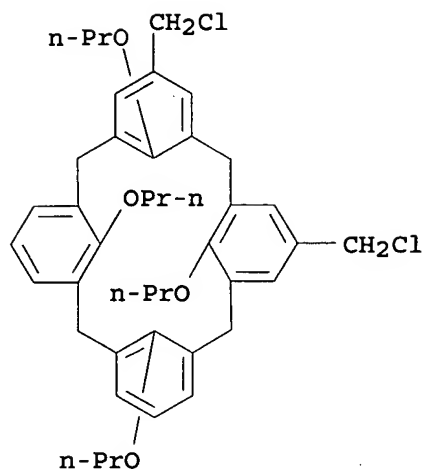
AB Two novel regioisomeric calix[4]arene derivs. (2 and 3), decorated  
with two aza[18]crown-6 units at vicinal (1,2) or diagonal (1,3)  
positions of the upper rim, were synthesized. The catalytic  
activities of their dinuclear Ba<sup>2+</sup> complexes were investigated in the  
ethanolysis of esters 8-11, endowed with a carboxylate anchoring  
group. Major results are as follows: (1) the two metal ions in the  
dinuclear catalysts work together in a cooperative fashion; (2) the  
vicinal calix[4]arene catalyst 2 is far superior to its diagonal  
regioisomer 3 in the reactions of all of the investigated esters; and  
(3) the distance between the carboxylate and ester carbonyl, which  
increases regularly from 8 to 11, influences reactivity of catalytic  
ester cleavage in a way that is decidedly suggestive of the importance  
of a good match between ester size and metal-to-metal distance.  
However, the superiority of the vicinal catalyst 2 relative to 3  
cannot be explained on the basis of the putative match of ester size  
to intermetal distance, thus providing an indication that addnl.,  
still poorly understood effects may contribute significantly to  
catalytic efficiency.

IT 792987-38-3P

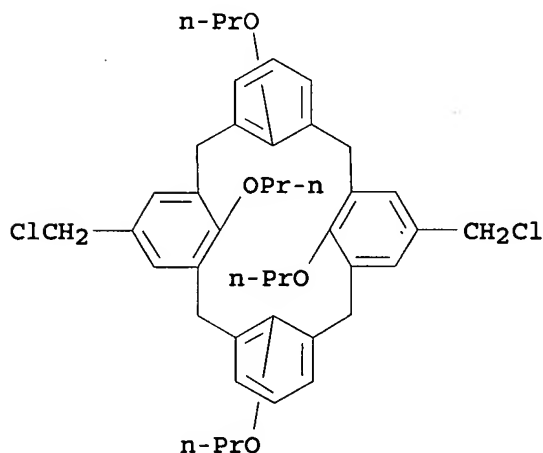
(dinuclear barium(II) complexes based on calix[4]arene scaffold as  
catalysts of acyl transfer)

RN 792987-38-3 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,11-bis(chloromethyl)-25,26,27,28-tetrapropoxy- (CA INDEX NAME)



IT 176098-86-5  
 (dinuclear barium(II) complexes based on calix[4]arene scaffold as  
 catalysts of acyl transfer)  
 RN 176098-86-5 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA  
 INDEX NAME)

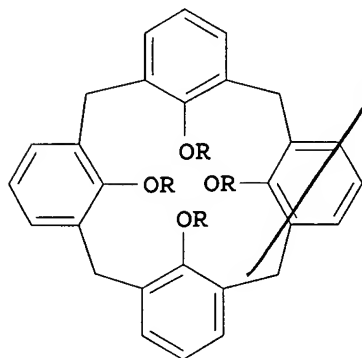


CC 22-4 (Physical Organic Chemistry)  
 Section cross-reference(s): 67  
 IT 792987-35-0P 792987-36-1P 792987-38-3P  
 (dinuclear barium(II) complexes based on calix[4]arene scaffold as  
 catalysts of acyl transfer)  
 IT 2092-17-3, Barium sulfocyanide 33941-15-0, 1-Aza[18]-crown-6  
 163121-51-5 176098-86-5 397255-67-3 397255-69-5  
 397255-71-9 602315-00-4 792987-37-2  
 (dinuclear barium(II) complexes based on calix[4]arene scaffold as  
 catalysts of acyl transfer)  
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
 RE FORMAT

L25 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:326420 HCAPLUS  
 DOCUMENT NUMBER: 140:339079  
 TITLE: Preparation of chloromethylated calix[4]arene mixtures for negative electron beam resists  
 INVENTOR(S): Momota, Junji; Oshima, Eiji  
 PATENT ASSIGNEE(S): Tokuyama Corp., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004123586	A	20040422	JP 2002-288430	20021001
PRIORITY APPLN. INFO.:			JP 2002-288430	20021001

OTHER SOURCE(S): CASREACT 140:339079; MARPAT 140:339079  
 ED Entered STN: 22 Apr 2004  
 GI



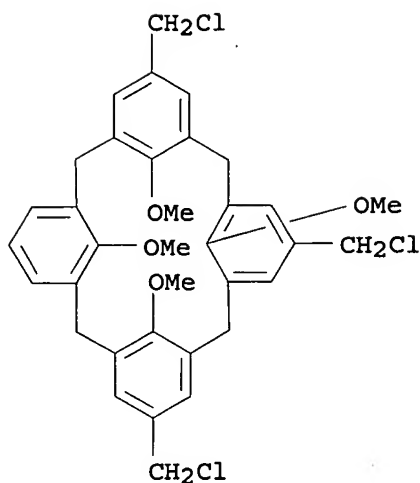
I

AB Calix[4]arenes I [R = (un)substituted C1-10 alkyl] are chloromethylated by HCl and HCHO in reaction systems containing 10-30 weight% H<sub>2</sub>O to give mixts. of tetrakis- and tris(chloromethylated) I. I (R = Me) (1.21 g) was treated with a mixture of 1,4-dioxane, AcOH, HCl, H<sub>3</sub>PO<sub>4</sub>, and 16 weight% H<sub>2</sub>O under reflux for 2 h to give 0.85 g 51:41 mixture of 5,11,17,23-tetrakis(chloromethyl)-I (R = Me) and 5,11,17-tris(chloromethyl)-I (R = Me).

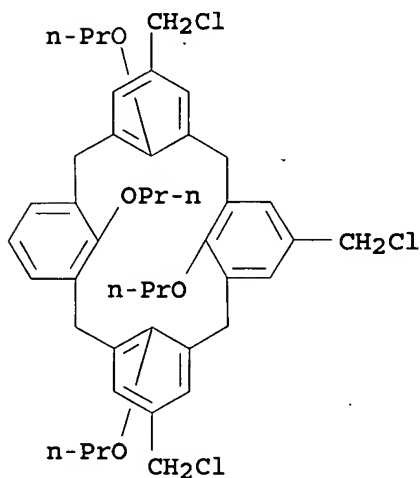
IT 673458-26-9P 680223-95-4P  
 (preparation of chloromethylated calix[4]arene mixts. for neg. electron beam resists)

RN 673458-26-9 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,11,17-tris(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)



RN 680223-95-4 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,11,17-tris(chloromethyl)-25,26,27,28-tetrapropoxy- (CA INDEX NAME)



IC ICM C07C041-22  
 ICS C07C043-225  
 CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 74  
 IT 139934-98-8P 325814-49-1P 673458-26-9P  
 680223-95-4P  
 (preparation of chloromethylated calix[4]arene mixts. for neg. electron  
 beam resists)

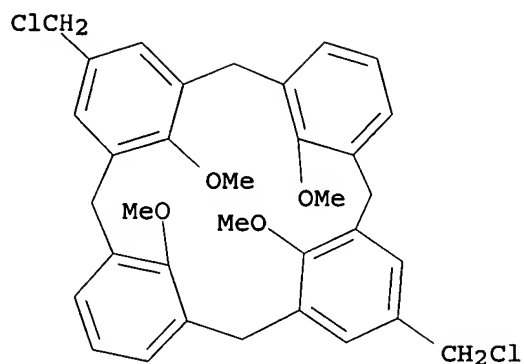
L25 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:220297 HCAPLUS  
 DOCUMENT NUMBER: 140:279682  
 TITLE: Resist and method of forming resist pattern  
 INVENTOR(S): Ochiai, Yukinori; Ishida, Masahiko; Fujita,  
 Junichi; Ogura, Takashi; Momoda, Junji; Oshima,

PATENT ASSIGNEE(S): Eiji  
 SOURCE: NEC Corporation, Japan; Tokuyama Corporation  
 PCT Int. Appl., 28 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004022513	A1	20040318	WO 2003-JP11284	20030904
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003261921	A1	20040329	AU 2003-261921	20030904
EP 1541543	A1	20050615	EP 2003-794216	20030904
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
US 20060127798	A1	20060615	US 2006-527068	20060104
PRIORITY APPLN. INFO.:			JP 2002-262314	A 20020909
			WO 2003-JP11284	W 20030904

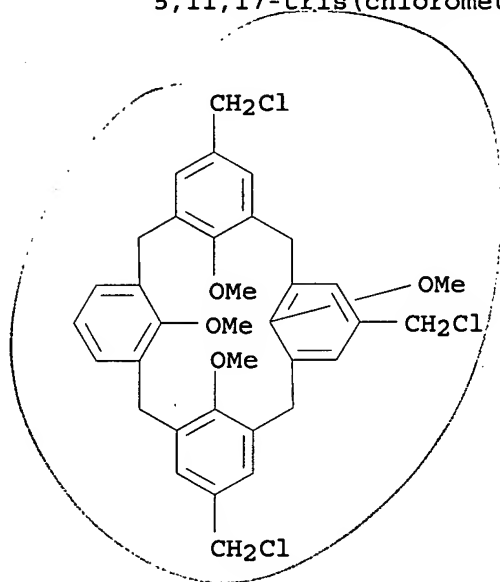
*Pre App.*

ED Entered STN: 19 Mar 2004  
 AB A resist comprising either tetrachloromethyltetramethoxycalix[4]arene or trichloromethyltetramethoxycalix[4]arene. The resist containing such a component is soluble in solvents that are favorable from the viewpoint of working environment, such as Et lactate (EL), propylene glycol monomethyl ether (PGME), propylene glycol monomethyl ether acetate (PGMEA), Et propionate, Bu acetate and 2-heptanone, and development can be conducted with not only these solvents but also tetramethylammonium hydroxide. Superhigh resolution of 8 nm can be obtained by exposing the resist to electron beams, and various materials can be microfabricated with the use of the resist as a mask. This resist enables providing a photosensitive resist material of high resolution which is soluble in solvents favorable from the viewpoint of working environment and thus can be developed by solvents favorable from the viewpoint of working environment; and a method of exposure or method of microfabrication with the use of the same.  
 IT 125065-73-8 673458-26-9 673458-27-0  
 (calixarene-containing electron beam resist and method of forming resist pattern for semiconductor device fabrication)  
 RN 125065-73-8 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosane-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 5,17-bis(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)



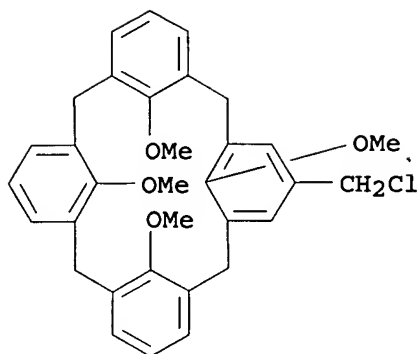
RN 673458-26-9 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,11,17-tris(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)



RN 673458-27-0 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5-(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)

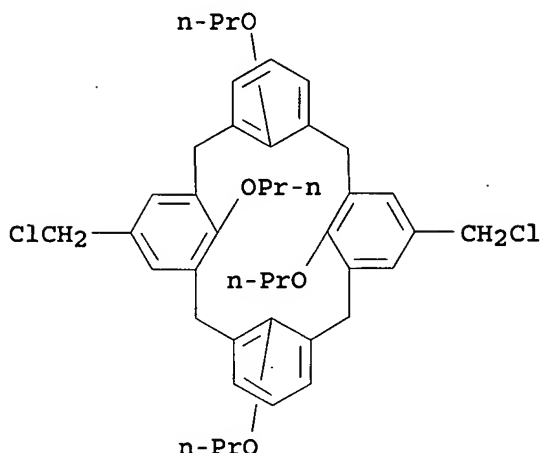


IC ICM C07C043-225  
 ICS G03F007-038; G03F007-004  
 CC 76-3 (Electric Phenomena)  
 Section cross-reference(s): 38  
 IT 125065-73-8 139934-98-8 673458-26-9  
 673458-27-0  
 (calixarene-containing electron beam resist and method of forming  
 resist pattern for semiconductor device fabrication)  
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
 RE FORMAT

L25 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:136147 HCAPLUS  
 DOCUMENT NUMBER: 140:321096  
 TITLE: Calix[4]arene-supported N-heterocyclic carbene  
 ligands as catalysts for Suzuki cross-coupling  
 reactions of chlorotoluene  
 AUTHOR(S): Frank, Markus; Maas, Gerhard; Schatz, Juergen  
 CORPORATE SOURCE: Division of Organic Chemistry I, University of  
 Ulm, Ulm, 89081, Germany  
 SOURCE: European Journal of Organic Chemistry (2004), (3),  
 607-613  
 CODEN: EJOCFK; ISSN: 1434-193X  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:321096  
 ED Entered STN: 19 Feb 2004  
 AB Stable N-heterocyclic carbenes are generated starting from  
 5,17-(bis-imidazolium)-substituted calix[4]arenes. Addition of Pd(OAc)<sub>2</sub>  
 to these carbenes leads to macrocyclic cis-palladium chelate complexes  
 in which the distal bridging of the upper rim leads to a strong  
 distortion of the calix[4]arene skeleton which was proven by X-ray  
 crystal structure determination Using an in-situ catalytic system consisting  
 of a calixarene-imidazolium salt, Cs<sub>2</sub>CO<sub>3</sub> as a base and a source of  
 palladium, a species is formed which can be used to catalyze the  
 Suzuki cross-coupling of 4-chloro toluene.  
 IT 176098-86-5P  
 (preparation of calixarene supported imidazole based carbene ligands as  
 catalysts for Suzuki cross-coupling reactions)  
 RN 176098-86-5 HCAPLUS  
 CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,



5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA INDEX NAME)



CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 29  
 IT 175912-54-6P 176098-86-5P 208984-10-5P 677353-71-8P  
 (preparation of calixarene supported imidazole based carbene ligands as  
 catalysts for Suzuki cross-coupling reactions)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
 RE FORMAT

L25 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:995678 HCAPLUS

DOCUMENT NUMBER: 140:163305

TITLE: Differential and Substrate-Selective Reactivity of  
 Calix[4]arene Derivatives with Cyclenyl-Zn(II)  
 Modifications at the Upper Rim

AUTHOR(S): Ozturk, Gulsum; Akkaya, Engin U.

CORPORATE SOURCE: Department of Chemistry, Middle East Technical  
 University, Ankara, TR-06531, Turk.

SOURCE: Organic Letters (2004), 6(2), 241-243

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:163305

ED Entered STN: 23 Dec 2003

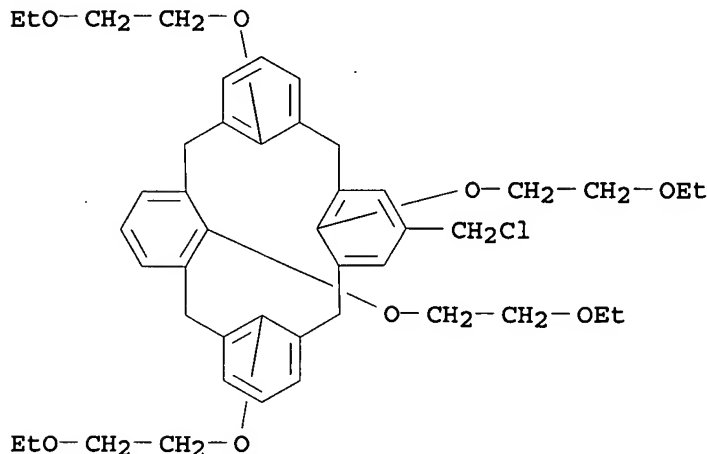
AB Novel cone conformation calix[4]arene derivs., carrying either one or  
 two cyclen (1,4,7,10-tetraazacyclododecane) moieties at the upper rim,  
 were synthesized. The hydrolytic activities of the Zn(II) complexes  
 of these calixarenes were studied. A surprising behavior was observed  
 with p-nitrophenyl stearate; whereas the bis-cyclenyl-2Zn(II) complex  
 showed negligible hydrolytic activity over the background, the  
 mononuclear complex showed a significant 400-fold rate increase at pH  
 8.5.

IT 656242-99-8P

(catalyst ligand; differential and substrate-selective reactivity  
 of calix[4]arene derivs. with cyclenyl-Zn(II) modifications at  
 upper rim)

RN 656242-99-8 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5-(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy)- (CA INDEX  
NAME)



CC 22-3 (Physical Organic Chemistry)  
Section cross-reference(s): 67, 78

IT 656242-99-8P 656243-03-7P  
(catalyst ligand; differential and substrate-selective reactivity  
of calix[4]arene derivs. with cyclenyl-Zn(II) modifications at  
upper rim)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L25 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:732444 HCAPLUS

DOCUMENT NUMBER: 140:375434

TITLE: Peptidocalix[4]arene self-assembled nanotubes

AUTHOR(S): Baldini, Laura; Sansone, Francesco; Casnati,  
Alessandro; Ugozzoli, Franco; Ungaro, Rocco

CORPORATE SOURCE: Dipartimento di Chimica Organica e Industriale,  
Universita degli Studi, Parma, I-43100, Italy

SOURCE: Journal of Supramolecular Chemistry (2003), Volume  
Date 2002, 2(1-3), 219-226  
CODEN: JSCOC9; ISSN: 1472-7862

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:375434

ED Entered STN: 18 Sep 2003

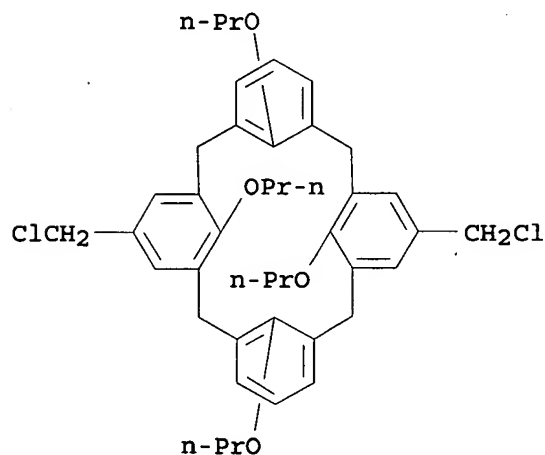
AB 5,17-Bis(N-benzyloxycarbonyl-L-alanylaminomethyl)-25,26,27,28-  
tetrapropoxycalix[4]arene was prepared and forms self-assembled  
nanotubes in the solid state through a two-dimensional network of  
hydrogen bonds between the amide chains of adjacent conformers. The  
crystal lattice is quite different from that of the analogous N-linked  
derivative which shows calix[4]arene macrocycles piled through van der  
Waals interactions.

IT 176098-86-5P, 5,17-Bis(chloromethyl)-25,26,27,28-  
tetrapropoxycalix[4]arene  
(preparation and self-assembled nanotube formation of

5,17-bis(N-benzyloxycarbonyl-L-alanylaminomethyl)-25,26,27,28-tetrapropoxycalix[4]arene)

RN 176098-86-5 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA  
INDEX NAME)



CC 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 28

IT 176098-86-5P, 5,17-Bis(chloromethyl)-25,26,27,28-tetrapropoxycalix[4]arene 196093-04-6P, 5,17-Bis(aminomethyl)-25,26,27,28-tetrapropoxycalix[4]arene 668481-66-1P  
(preparation and self-assembled nanotube formation of  
5,17-bis(N-benzyloxycarbonyl-L-alanylaminomethyl)-25,26,27,28-tetrapropoxycalix[4]arene)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L25 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:787065 HCAPLUS

DOCUMENT NUMBER: 138:32346

TITLE: Synthesis and Characterization of Diametrically  
Substituted Tetra-O-n-butylcalix[4]arene Ligands  
and Their Chelated Complexes of Titanium,  
Molybdenum, and Palladium

AUTHOR(S): Evans, Daniel R.; Huang, Mingsheng; Fetting, James C.; Williams, Tracie L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry,  
University of Maryland, College Park, MD, 20742,  
USA

SOURCE: Inorganic Chemistry (2002), 41(23), 5986-6000  
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:32346

ED Entered STN: 16 Oct 2002

AB The ligation properties of three new upper-rim-substituted  
calix[4]arene ligands, 5,17-bis(hydroxymethyl)-tetra-n-

butoxycalix[4]arene ((HOCH<sub>2</sub>)<sub>2</sub>Bu<sub>4</sub>Clx, 7), 5,17-bis((diphenylphosphinito)methoxy)-tetra-n-butoxycalix[4]arene ((PPh<sub>2</sub>OCH<sub>2</sub>)<sub>2</sub>Bu<sub>4</sub>Clx, 8), and 5,17-bis((diphenylphosphino)methyl)-tetra-n-butoxycalix[4]arene ((PPh<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>Bu<sub>4</sub>Clx, 10) are reported herein. The newly prepared compds. differ from previously reported diametrically substituted calix[4]arene derivs. in that the lower-rim substituent was Bu. The presence of this lower-rim substituent did not reduce the inherent crystallinity of these complexes as purification of all materials occurred via simple crystns. The key precursor for the syntheses of 8 and 10 was 7, acquisition of which occurred in six steps starting from tetra-tert-butylcalix[4]arene, 1. Calix[4]arene derivs. include, tetra-n-butoxycalix[4]arene (Bu<sub>4</sub>Clx, 3), 5,11,17,23-tetrabromo-tetra-n-butoxycalix[4]arene (Br<sub>4</sub>-Bu<sub>4</sub>Clx, 4), 5,17-dibromo-tetra-n-butoxycalix[4]arene (Br<sub>2</sub>-Bu<sub>4</sub>Clx, 5), 5,17-bis(formyl)-tetra-n-butoxycalix[4]arene ((CHO)<sub>2</sub>-Bu<sub>4</sub>Clx, 6), and 5,17-bis(chloromethyl)-tetra-n-butoxycalix[4]arene ((ClCH<sub>2</sub>)<sub>2</sub>-Bu<sub>4</sub>Clx, 9), all of which were synthesized using modifications of existing procedures. Characterization of all compds. occurred, when possible, using <sup>1</sup>H, <sup>13</sup>C, and <sup>31</sup>P NMR, elemental analyses, FAB-MS, ESI-MS, FTIR, and x-ray crystallog. The solid-state structures of all calix[4]arene intermediates and ligands showed that the annulus adopted the pinched-cone conformation in which the average C(5)···C(17) intraannular separation was 4.5 ± 0.4 Å. Reaction of 7 with CpTiMe<sub>3</sub> yielded the cis-chelate, CpTi(Me)[(OCH<sub>2</sub>)<sub>2</sub>Bu<sub>4</sub>Clx] (11), quant. Data obtained using ESI-MS (pos.-ion mode) confirmed the monomer formulation showed above, and <sup>1</sup>H NMR spectra provided sufficient information to deduce the nature of the Ti coordination sphere. Reaction of 8 with cis-Cl<sub>2</sub>Pd(NCPh)<sub>2</sub> in refluxing benzene afforded cis-Cl<sub>2</sub>Pd[(PPh<sub>2</sub>OCH<sub>2</sub>)<sub>2</sub>Bu<sub>4</sub>Clx] (12) in good yields. The monomeric identity of 12 was verified by both x-ray crystallog. and pos.-ion ESI-MS. The cis-bidentate calix[4]arene ligand did not undergo any noticeable contortion upon chelation of the PdCl<sub>2</sub> fragment. Acid-promoted decomposition of 12 occurred in the presence of adventitious HCl and gaseous HCl, and the products of this decomposition were 9 and [μ<sub>2</sub>-ClPd(PPh<sub>2</sub>OH)(PPh<sub>2</sub>O)]<sub>2</sub>. Chelates of 8 that contained Mo(CO)<sub>3</sub>L (L = NCMe (14a), NCET (14b), and CO (14c)) showed that the mode of coordination was relatively insensitive to the identity of the metal. x-ray crystallog. afforded views of the solid-state structures of 14b,c and, like 12, showed that the Mo(CO)<sub>3</sub>L fragment resided above the pinched-cone of the calix[4]arene. <sup>1</sup>H NMR revealed that C-H/π interactions existed between L (14a,b) and a Ph ring of the coordinated phosphinite. Finally, the bis(diphenylphosphine)calix[4]arene ligand (10) readily coordinated the Mo(CO)<sub>3</sub>L species, but the reaction did not go to completion, as evidenced by <sup>1</sup>H NMR, even after a 5 day reaction time. Probably the product is similar to that observed for 12 and 14, but the incomplete reaction complicated attempts to obtain pure material and prohibited definitive assignment of the coordination array.

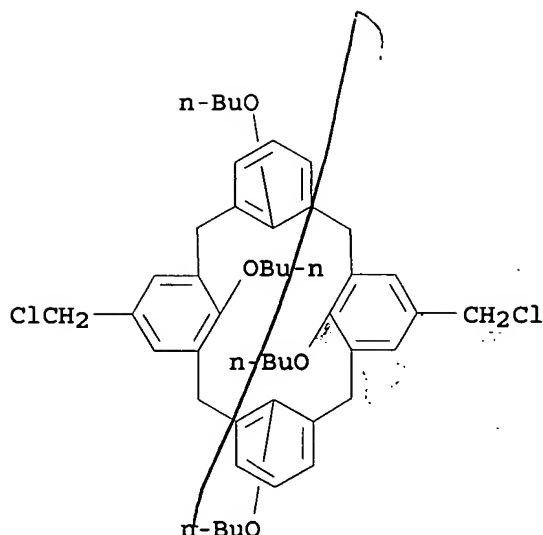
IT 477842-01-6

(reaction with diphenylphosphine)

RN 477842-01-6 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-

1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
25,26,27,28-tetrabutoxy-5,17-bis(chloromethyl)- (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 28, 29, 75

IT 477842-01-6

(reaction with diphenylphosphine)

REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:207118 HCAPLUS

DOCUMENT NUMBER: 136:385933

TITLE: Calix[4]arenes Linked to Multiple Bidentate N-Donors: Potential Ligands for Synthetic Modeling of Multinuclear Metalloenzymes

AUTHOR(S): Spencer, Douglas J. E.; Johnson, Bryan J.; Johnson, Brian J.; Tolman, William B.

CORPORATE SOURCE: Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota, Minneapolis, MN, 55455, USA

SOURCE: Organic Letters (2002), 4(8), 1391-1393  
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

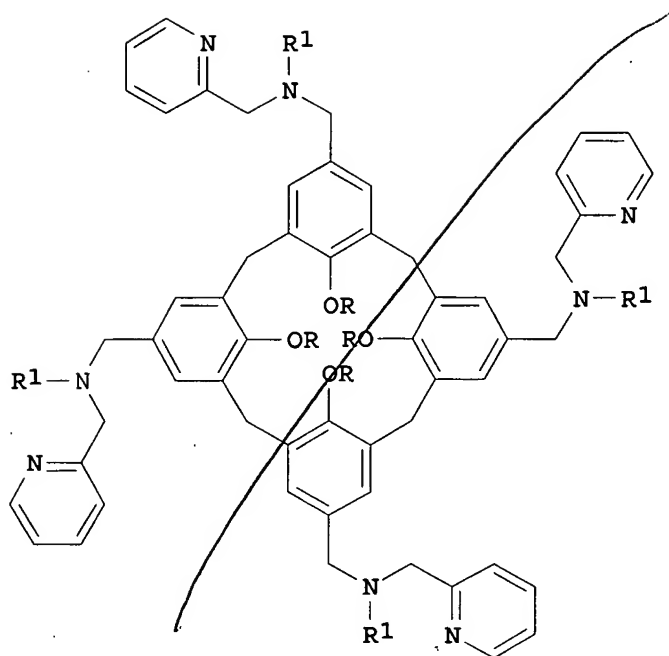
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:385933

ED Entered STN: 20 Mar 2002

GI



I

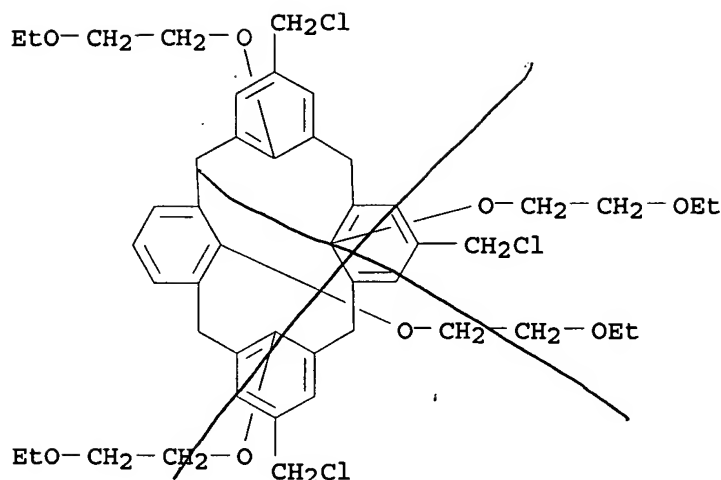
AB Calixarenes incorporating three or four bidentate diamines or heterocyclylmethanamines attached at the "upper rim" such as I ( $R = \text{EtOCH}_2\text{CH}_2$ ;  $R_1 = \text{Me}_2\text{CH}$ ,  $\text{PhCH}_2$ ) were prepared via practical protocols. Alkylation of a tetrahydroxycalix[4]arene with excess 2-ethoxyethyl bromide and sodium hydride gave a tetra(2-ethoxyethyl)calixarene; tetraformylation, reduction of the aldehyde groups with sodium borohydride, and chlorination with thionyl chloride gave a tetrachloromethyl calixarene which is a versatile intermediate for the preparation of substituted calixarenes. An analogous method using a trisformylation reaction gave the corresponding tris(chloromethyl)calixarene. Substitution of the chloromethyl groups with amines such as  $N,N,N'$ -trimethyl-1,3-propanediamine,  $N$ -isopropyl-2-pyridinemethanamine, and  $N$ -isopropyl-2-quinolinemethanamine yielded calixarenes such as I ( $R = \text{EtOCH}_2\text{CH}_2$ ;  $R_1 = \text{Me}_2\text{CH}$ ,  $\text{PhCH}_2$ ). Calixarenes such as I were designed as potential analogs of multinuclear metalloenzymes. The crystal structure of I ( $R = \text{EtOCH}_2\text{CH}_2$ ;  $R_1 = \text{PhCH}_2$ ) was determined by X-ray crystallog.

IT 426836-42-2P

(preparation of tri- and tetra-substituted calixarene substituted with bidentate amine moieties as potential mimics of multinuclear metalloenzymes)

RN 426836-42-2 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,11,17-tris(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy)- (CA  
INDEX NAME)



CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 75  
 IT 18081-89-5P 58669-30-0P 105487-97-6P 154459-66-2P 155057-44-6P  
 166940-40-5P 426836-40-0P 426836-41-1P 426836-42-2P  
 (preparation of tri- and tetra-substituted calixarene substituted with  
 bidentate amine moieties as potential mimics of multinuclear  
 metalloenzymes)

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
 RE FORMAT

L25 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:372682 HCAPLUS

DOCUMENT NUMBER: 135:211119

TITLE: Metal complexes based on an upper rim  
 calix[4]arene phosphine ligand

AUTHOR(S): Fang, X.; Scott, B. L.; Watkin, J. G.; Carter, C.  
 A. G.; Kubas, G. J.

CORPORATE SOURCE: Los Alamos National Laboratory, Chemistry  
 Division, Los Alamos, NM, 87544, USA

SOURCE: Inorganica Chimica Acta (2001), 317(1,2), 276-281  
 CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:211119

ED Entered STN: 24 May 2001

AB A new upper rim phosphacalix[4]arene 5,17-bis(diphenylphosphinomethyl)-  
 25,26,27,28-tetrapropoxycalix[4]arene (I) was prepared starting from  
 com. available tert-Bu calix[4]arene. Treatment of I with (COD)PdMeCl  
 and (COD)PtCl<sub>2</sub> gives polymeric phosphine-coordinated Pd(II) and Pt(II)  
 species, resp.; I reacts with [(COD)RhCl]<sub>2</sub> to give a dirhodium complex  
 that is an active catalyst for the hydroformylation of 1-octene and  
 styrene.

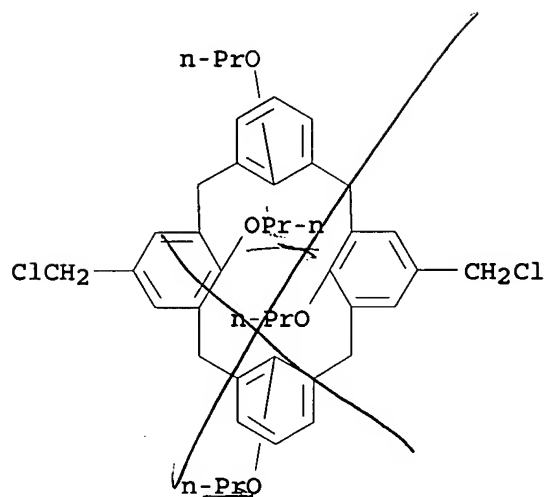
IT 176098-86-5P

(preparation and phosphination with diphenylphosphine)

RN 176098-86-5 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA

INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 23, 75

IT 176098-86-5P

(preparation and phosphination with diphenylphosphine)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L25 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:158970 HCAPLUS

DOCUMENT NUMBER: 132:250863

TITLE: Guest inclusion properties of a novel cage  
molecule composed of two calix[4]arenes

AUTHOR(S): Araki, Koji; Hayashida, Hiromi

CORPORATE SOURCE: Department of Applied Chemistry, Kyushu Institute  
of Technology, Faculty of Engineering, Kitakyushu,  
804-8550, Japan

SOURCE: Tetrahedron Letters (2000), 41(8), 1209-1213

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 10 Mar 2000

AB The bis-calix[4]arene was synthesized by connecting the upper rims with  
two spacers. The inclusion ability and the selectivity for various  
quaternary ammonium ions were enhanced due to the cooperative action  
of the cation- $\pi$  interaction in the two bowl-shaped calix[4]arenes.  
The very slow dynamic process during complexation and decomplexation  
and the separation of the cationic guest and the counter anion were caused  
by encapsulation of the bis-calix[4]arene.

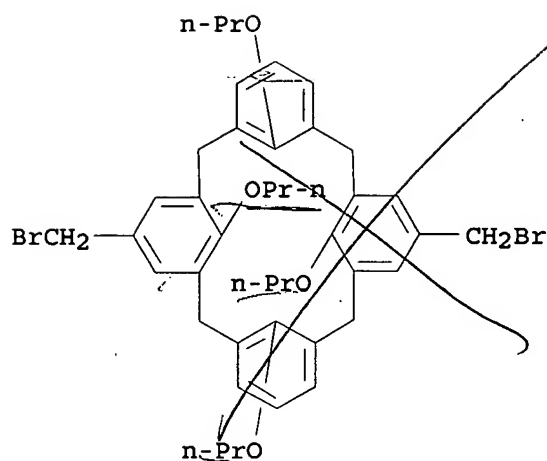
IT 262590-47-6P

(intermediates in synthesis of cage mol. composed of two  
calix[4]arene units)

RN 262590-47-6 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(bromomethyl)-25,26,27,28-tetrapropoxy- (CA INDEX NAME)





CC 22-10 (Physical Organic Chemistry)

Section cross-reference(s): 68

IT 175019-04-2P 261634-82-6P 262590-47-6P

(intermediates in synthesis of cage mol. composed of two calix[4]arene units)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:105652 HCAPLUS

DOCUMENT NUMBER: 128:192633

TITLE: Synthesis of multiply-connected 1,3-alternate-calix[4]arenes. A novel approach to synthetic "nano-tubes"

AUTHOR(S): Ikeda, Atsushi; Kawaguchi, Masaru; Shinkai, Seiji

CORPORATE SOURCE: Department of Chemical Science & Technology, Faculty of Engineering, Kyushu University, Fukuoka, 812, Japan

SOURCE: Anales de Quimica International Edition (1997), 93(6), 408-414

CODEN: AQIEFZ

PUBLISHER: Springer-Verlag Iberica

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 21 Feb 1998

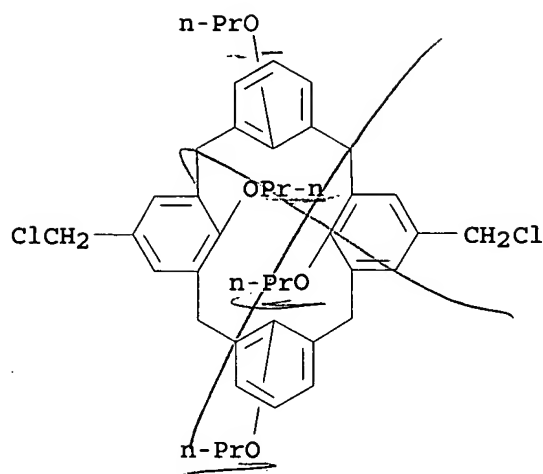
AB Certain metal cations can oscillate between two metal-binding sites in a 1,3-alternate-calix[4]arene through its  $\pi$ -basic cavity. Hence, it is expected that one-dimensional multiple connection of 1,3-alternate-calix[4]arenes provides novel synthetic "nano-tubes" for metal cation tunneling. A synthetic approach to five multiply-connected 1,3-alternate-calix[4]arenes is reported.

IT 176098-86-5P

(synthesis of multiply-connected calix[4]arene nano-tubes)

RN 176098-86-5 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA INDEX NAME)



CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 161058-40-8P 163121-51-5P 172472-58-1P 175019-04-2P

176098-86-5P 190390-28-4P 203579-88-8P

(synthesis of multiply-connected calix[4]arene nano-tubes)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L25 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:23031 HCAPLUS

DOCUMENT NUMBER: 128:114936

TITLE: Synthesis and metal-binding properties of  
[60]fullerene-linked calix[4]arenes: an approach  
to 'exohedral metallofullerenes'

AUTHOR(S): Kawaguchi, Masaru; Ikeda, Atsushi; Shinkai, Seiji

CORPORATE SOURCE: Faculty of Engineering, Department of Chemical  
Science + Technology, Kyushu University, Fukuoka,  
812, Japan

SOURCE: Journal of the Chemical Society, Perkin  
Transactions 1: Organic and Bio-Organic Chemistry  
(1998), (2), 179-184

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 16 Jan 1998

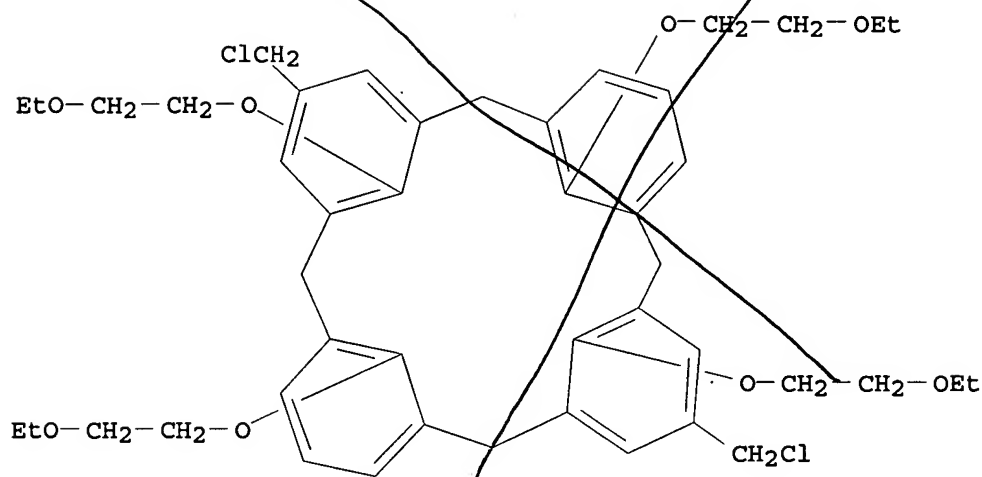
AB Fullerenocalixarenes in which [60]fullerene is covalently linked  
through two ionophoric chains to a cone-calix[4]arene (I) or to a  
1,3-alternate calix[4]arene (II) have been synthesized for the first  
time. Although the absorption spectrum of II is scarcely changed upon  
addition of metal cations, that of I is affected by added Li<sup>+</sup>, Na<sup>+</sup> and  
Ag<sup>+</sup>, indicating the formation of exohedral [60]fullerene-metal  
complexes.

IT 166665-14-1P

(preparation and metal-binding properties of [60]fullerene-linked  
calix[4]arenes)

RN 166665-14-1 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosane-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy) - (CA  
INDEX NAME)



CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
 IT 99685-96-8DP, Fullerene C<sub>60</sub>, calixarene derivs. 156856-43-8P  
 166665-14-1P 166940-42-7P 177412-47-4P 177412-49-6P  
 201743-82-0P 201743-83-1P 201743-84-2P  
 (preparation and metal-binding properties of [60]fullerene-linked calix[4]arenes)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:155212 HCAPLUS

DOCUMENT NUMBER: 124:316715

ORIGINAL REFERENCE NO.: 124:58733a,58736a

TITLE: Upper-Rim Urea-Derivatized Calix[4]arenes as

Neutral Receptors for Monocarboxylate Anions

AUTHOR(S): Casnati, Alessandro; Fochi, Mariacristina; Minari, Patrizia; Pochini, Andrea; Reggiani, Massimo; Ungaro, Rocco

CORPORATE SOURCE: Dipartimento Chimica Organica Industriale, Universita Parma, Parma, I-43100, Italy

SOURCE: Gazzetta Chimica Italiana (1996), 126(2), 99-106

CODEN: GCITA9; ISSN: 0016-5603

PUBLISHER: Societa Chimica Italiana

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:316715

ED Entered STN: 16 Mar 1996

AB Several new anion receptors were synthesized by introducing one or two urea or thiourea units at the upper rim of calix[4]arenes, blocked in the cone conformation. One difunctionalized receptor showed selectivity in the recognition of acetate anion, which interacts with the two urea units through four hydrogen bonds. Two monofunctionalized receptors complexed more strongly with aromatic carboxylates or butyrate anion since the primary hydrogen bonding contacts were strengthened by weak  $\pi/\pi$  or  $\text{CH}_3/\pi$  host-guest interactions.

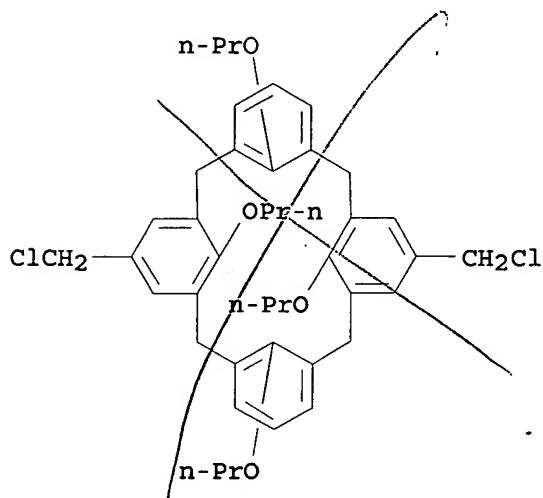
IT 176098-86-5P 176098-97-8P

(upper-rim urea-derivatized calix[4]arenes as neutral receptors for

carboxylate anions)

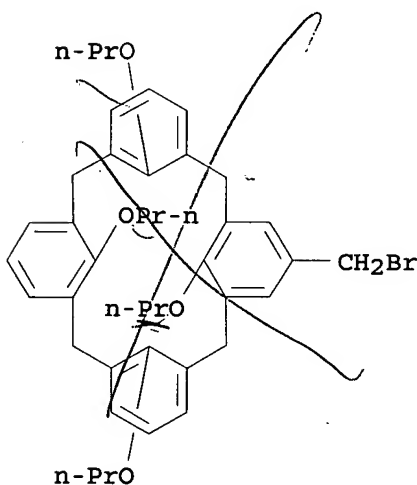
RN 176098-86-5 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA  
INDEX NAME)



RN 176098-97-8 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5-(bromomethyl)-25,26,27,28-tetrapropoxy-, stereoisomer (CA INDEX  
NAME)



CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 22

IT 176098-84-3P 176098-85-4P 176098-86-5P 176098-87-6P  
176098-88-7P 176098-89-8P 176098-90-1P 176098-91-2P  
176098-92-3P 176098-95-6P 176098-96-7P 176098-97-8P  
176298-99-0P 176299-00-6P

(upper-rim urea-derivatized calix[4]arenes as neutral receptors for  
carboxylate anions)

L25 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:397619 HCAPLUS

DOCUMENT NUMBER: 123:143421

ORIGINAL REFERENCE NO.: 123:25533a,25536a

TITLE: Direct Regioselective Formylation of Tetraalkoxycalix[4]arenes Fixed in the Cone Conformation and Synthesis of New Cavitands

AUTHOR(S): Arduini, Arturo; Fanni, Stefano; Manfredi, Giuseppe; Pochini, Andrea; Ungaro, Rocco; Sicuri, Anna R.; Ugozzoli, Franco

CORPORATE SOURCE: Dipartimento di Chimica Organica e Industriale, Universita' Viale delle Scienze, Parma, 43100, Italy

SOURCE: Journal of Organic Chemistry (1995), 60(5), 1448-53

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:143421

ED Entered STN: 08 Mar 1995

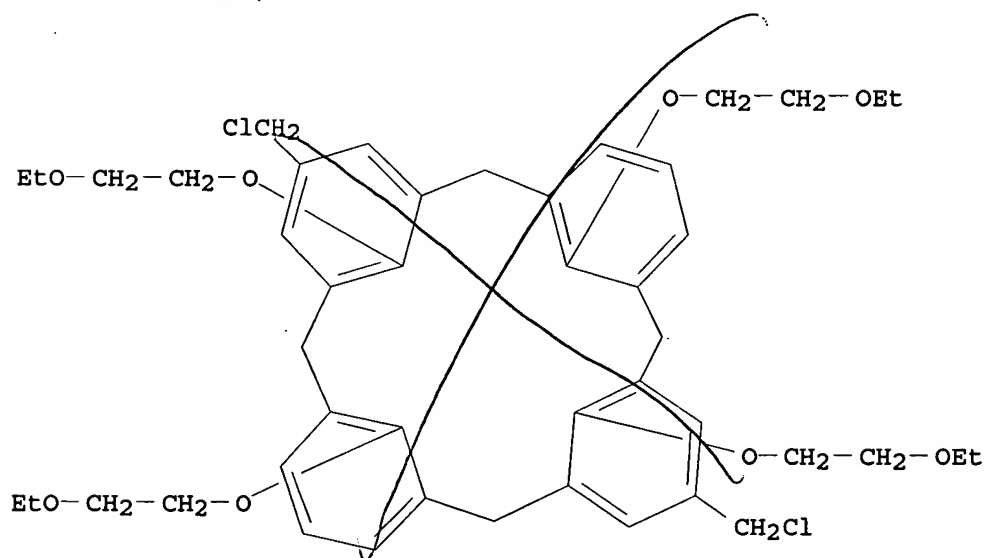
AB Regioselectivity of the formylation of tetraalkoxycalix[4]arenes fixed in the cone conformation has been studied. Direct, diametrical (1,3) diformylation of calix[4]arenes having four chelating chains at the lower rim has been achieved. Simple tetraalkoxycalix[4]arenes produce a mixture of diametrical (1,3) and proximal (1,2) diformylated products. The (1,3) functionalized compds. have been used for the synthesis of double calix[4]arenes linked via the upper rim. The residual mobility of these cone conformers is indicated by the x-ray crystal structure of one compound, which shows a flattened cone conformation, and by the reactive behavior of two 1,3-bis(hydroxymethyl) derivs., which give very distorted 1,3-bridged compds. through an intramol. cyclization process.

IT 166665-14-1P

(preparation of)

RN 166665-14-1 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetrakis(2-ethoxyethoxy)- (CA  
INDEX NAME)



CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 IT 156856-43-8P 166665-09-4P 166665-10-7P 166665-11-8P  
 166665-13-0P 166665-14-1P 166665-15-2P 166665-16-3P  
 166665-17-4P 166665-19-6P 166665-20-9P 166940-38-1P  
 166940-39-2P 166940-40-5P 166940-43-8P  
 (preparation of)

L25 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:498356 HCAPLUS

DOCUMENT NUMBER: 121:98356

ORIGINAL REFERENCE NO.: 121:17415a,17418a

TITLE: Synthesis of and amine recognition with a  
 Cu(II)-bridged biscalic[4]arene

AUTHOR(S): Fujimoto, Kiyoshi; Shinkai, Seiji

CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan

SOURCE: Tetrahedron Letters (1994), 35(18), 2915-18

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 20 Aug 1994

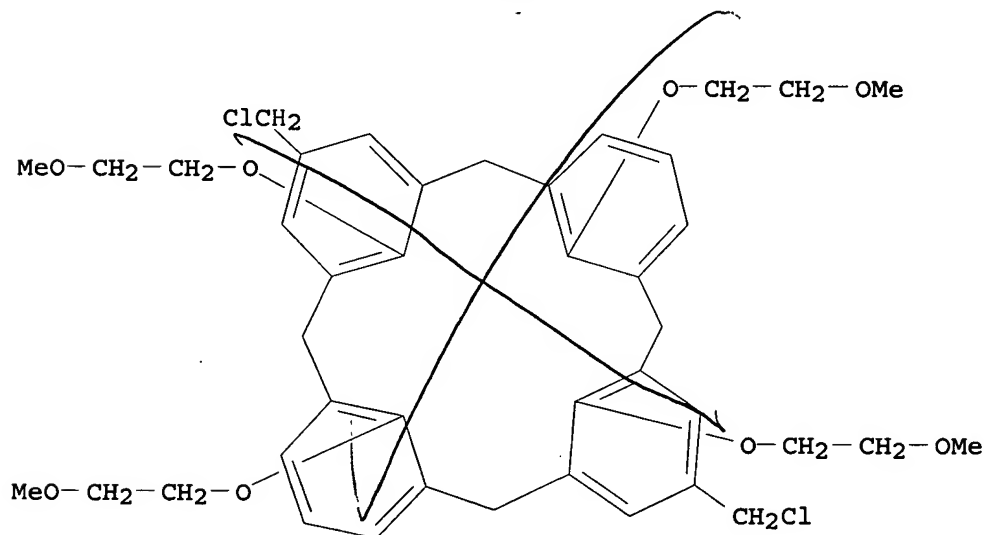
GI For diagram(s), see printed CA Issue.

AB A biscalic[4]arene I in which the upper rims are linked by 2  
 Cu(II)-chelate complexes was synthesized. This is a novel method for  
 the synthesis of biscalic[4]arenes using the self-association nature of  
 metal ligands. I recognized diamine substrates using a cavity  
 composed to 2 Cu(II)-chelate complexes.

IT 155939-39-2P  
 (preparation and reaction of, with acetylacetonate)

RN 155939-39-2 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-  
 1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
 5,17-bis(chloromethyl)-25,26,27,28-tetrakis(2-methoxyethoxy)-,  
 stereoisomer (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 68

IT 155939-39-2P

(preparation and reaction of, with acetylacetonate)

L25 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:163400 HCAPLUS

DOCUMENT NUMBER: 114:163400

ORIGINAL REFERENCE NO.: 114:27621a,27624a

TITLE: Upper rim calixcrowns: elucidation of the mechanism of conformational interconversion of calix[4]arenes by quantitative 2-D EXSY NMR spectroscopy

AUTHOR(S): Van Loon, Jan Dirk; Groenen, Leo C.; Wijmenga, Sybren S.; Verboom, Willem; Reinhoudt, David N.  
CORPORATE SOURCE: Dep. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.

SOURCE: Journal of the American Chemical Society (1991), 113(7), 2378-84

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:163400

ED Entered STN: 03 May 1991

GI For diagram(s), see printed CA Issue.

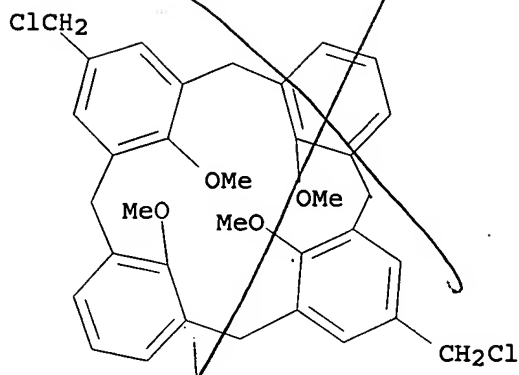
AB Tetramethoxycalix[4]arenes I (n = 0-4) bridged by a polyether chain at the upper rim (upper rim calixcrowns) were synthesized by reaction of 5,17-bis(chloromethyl)-25,26,27,28-tetramethoxycalix[4]arene with poly(oxyethylene) glycols of different length (mono to penta). In CDCl<sub>3</sub> solution at -20°, these compds. exist as a mixture of two conformations, viz. the partial cone (P) and the cone (C). The P/C ratio varies between 4.0 and 1.7 depending on the length of the bridge. The upper rim calixcrowns are flexible mols. according to temperature-dependent <sup>1</sup>H NMR. For the first time the mechanism of conformational interconversion of calix[4]arenes I (n = 0, 1) was elucidated by quant. 2-D EXSY NMR spectroscopy. It proves that there are two different pathways (a slow and a fast process) by which the two P conformational topomers can interconvert. One interconversion proceeds via C (slow process), and the other process proceeds most likely via a short-lived 1,3-alternate intermediate (A) (fast process). The rate consts. for both pathways were determined; calix[4]crown-2 I (n = 0), k<sub>PA</sub> = 0.58, k<sub>PC</sub> = 0.054, and k<sub>CP</sub> = 0.27 s<sup>-1</sup> at 298 K, and calix[4]crown-3 I (n = 1), k<sub>PA</sub> = 5.4, k<sub>PC</sub> = 0.07, and k<sub>CP</sub> = 0.18 s<sup>-1</sup> at 253 K. The overall rate diminishes dramatically going from a nine-atom bridge in I (n = 1) to a six-atom bridge in I (n = 0). Furthermore, shortening of the bridge has a much larger decelerating effect on the P → A than on the P → C process.

IT 125065-73-8

(cycloaddn. of, with polyethylene glycols)

RN 125065-73-8 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)



CC 22-10 (Physical Organic Chemistry)  
 IT 125065-73-8  
 (cycloaddn. of, with polyethylene glycols)

L25 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:571640 HCAPLUS

DOCUMENT NUMBER: 113:171640

ORIGINAL REFERENCE NO.: 113:29109a,29112a

TITLE: Selective functionalization of calix[4]arenes at the upper rim

AUTHOR(S): Van Loon, Jan Dirk; Arduini, Arturo; Coppi, Laura; Verboom, Willem; Pochini, Andrea; Ungaro, Rocco; Harkema, Sybolt; Reinhoudt, David N.

CORPORATE SOURCE: Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.

SOURCE: Journal of Organic Chemistry (1990), 55(21), 5639-46

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:171640

ED Entered STN: 09 Nov 1990

AB Methods are described for the selective diametrical functionalization of calix[4]arenes at the upper rim, either by the selective removal of the p-tert-Bu groups and subsequent substitution at the free phenol rings or by selective reactions at the phenol rings of dialkoxycalix[4]arenes without the tert-Bu groups. This includes selective mercuration and the synthesis of 5,17-di-tert-butyl-26,28-dimethoxy-11,23-diphenylcalix[4]arene of which the crystal structure is described. The first synthesis of macrocyclic diquinones derived from calix[4]arenes (calix[4]diquinones) is described.

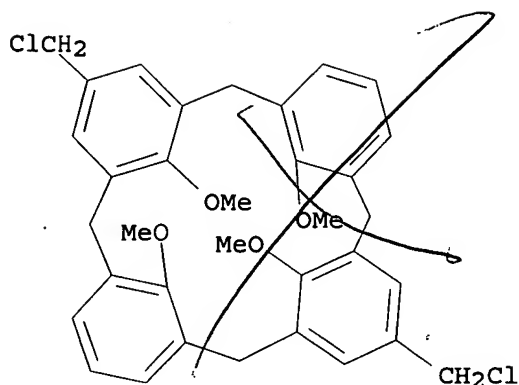
IT 129568-41-8P

(preparation and rearrangement of)

RN 129568-41-8 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 5,17-bis(chloromethyl)-25,26,27,28-tetramethoxy-, stereoisomer (CA INDEX NAME)





CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 75

IT 125065-62-5P 129492-34-8P 129568-37-2P 129568-41-8P  
129568-42-9P

(preparation and rearrangement of)

L25 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:76575 HCAPLUS

DOCUMENT NUMBER: 112:76575

ORIGINAL REFERENCE NO.: 112:13075a, 13078a

TITLE: Selective functionalization of calix[4]arenes at the upper rim

AUTHOR(S): Van Loon, J. D.; Arduini, A.; Verboom, W.; Ungaro, R.; Van Hummel, G. J.; Harkema, S.; Reinhoudt, D. N.

CORPORATE SOURCE: Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.

SOURCE: Tetrahedron Letters (1989), 30(20), 2681-4  
CODEN: TELEAY, ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:76575

ED Entered STN: 03 Mar 1990

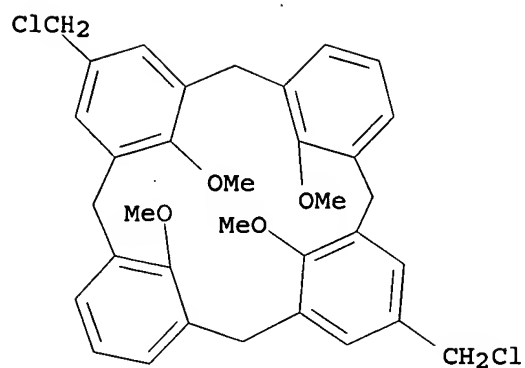
AB Methods are described for the selective diametrical functionalization of calix[4]arenes at the upper rim by transfer of functionality and selective substitutions at the para positions of the phenol rings. The crystal structure of 26,28-dimethoxy-11,23-dinitrocalix[4]arene is described.

IT 125065-73-8P

(preparation of)

RN 125065-73-8 HCAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-  
1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene,  
5,17-bis(chloromethyl)-25,26,27,28-tetramethoxy- (CA INDEX NAME)



CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 75  
IT 125065-63-6P 125065-69-2P 125065-73-8P 125065-74-9P  
125065-75-0P 125065-78-3P 125065-79-4P 125065-81-8P  
(preparation of)

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(FILE 'HOME' ENTERED AT 07:47:18 ON 30 MAY 2008)

FILE 'HCAPLUS' ENTERED AT 07:47:28 ON 30 MAY 2008

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SEL RN

FILE 'REGISTRY' ENTERED AT 07:47:43 ON 30 MAY 2008

L2 10 SEA ABB=ON PLU=ON (105-37-3/BI OR 110-43-0/BI OR  
123-86-4/BI OR 125065-73-8/BI OR 1320-67-8/BI OR 139934-98-  
8/BI OR 673458-26-9/BI OR 673458-27-0/BI OR 84540-57-8/BI  
OR 97-64-3/BI)  
L3 4 SEA ABB=ON PLU=ON L2 AND 1-100/NR  
L4 1 SEA ABB=ON PLU=ON 139934-98-8/RN  
L5 0 SEA ABB=ON PLU=ON 139934-98-8/CRN  
L6 1 SEA ABB=ON PLU=ON 125065-73-8/RN  
L7 0 SEA ABB=ON PLU=ON 125065-73-8/CRN

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L8 11 SEA ABB=ON PLU=ON L4  
L9 4 SEA ABB=ON PLU=ON L6

FILE 'REGISTRY' ENTERED AT 07:51:24 ON 30 MAY 2008

L10 STR  
L11 2 SEA SSS SAM L10  
L12 STR L10  
L13 1 SEA SSS SAM L12  
L14 528 SEA SSS FUL L12  
L15 4 SEA ABB=ON PLU=ON L14 AND L2  
SAV L14 LEE068/A  
L16 STR L10  
L17 1 SEA SUB=L14 SSS SAM L16  
L18 27 SEA SUB=L14 SSS FUL L16  
SAV L18 LEE068A/A  
L19 STR L10  
L20 3 SEA SUB=L14 SSS SAM L19  
L21 19 SEA SUB=L14 SSS FUL L19  
SAV L21 LEE068B/A  
L22 16 SEA ABB=ON PLU=ON L21 NOT ( ISOBENZOFURANONE OR  
PYRAN-6-ONE)  
L23 482 SEA ABB=ON PLU=ON L14 NOT (L18 OR L21)

FILE 'HCAPLUS' ENTERED AT 08:27:19 ON 30 MAY 2008

L24 64 SEA ABB=ON PLU=ON L18  
L25 24 SEA ABB=ON PLU=ON L22

FILE 'REGISTRY' ENTERED AT 08:28:38 ON 30 MAY 2008

L26 6 SEA ABB=ON PLU=ON L23 AND PMS/CI